Reading list

- **Reproducible Computational Workflows with Continuous Analysis**, Brett K. Beaulieu-Jones & Casey S. Greene. bioRxiv 056473
- **Introducing eLife's first computationally reproducible article**
- **Reproducible Document Stack: towards a scalable solution for reproducible articles**
- **The Turing Way** – a lightly-opinionated guide to reproducible data science; led by Kirstie Whitaker (@kirstie_j #TheTuringWay)
- **Making Reproducibility Reproducible** – written by the Gigantum Team @gigantumscience
- **Reproducibility: automated.**
- **2014: What scientific idea is ready for retirement?** (defining different types of reproducibility).
- **The possibility and desirability of replication in the humanities**. Rik Peels & Lex Boulter. *Palgrave Communications* 4, 95 (2018).
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https://doi.org/10.6084/m9.figshare.8299226
Reproducible Computational Workflows with Continuous Analysis

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UNIGE-CERN OAI11, June 20, 2019, Geneva
“Reproducing experiments is vital to science.”
Beaulieu-Jones & Greene, 2016

“Scientific results and evidence are strengthened if they are reproduced and confirmed by several independent researchers.”
The Turing Way Book

Reproducible Computational Workflows with Continuous Analysis, Brett K. Beaulieu-Jones, Casey S. Greene, bioRxiv 056473; doi: https://doi.org/10.1101/056473
The Turing Way, a lightly-opinionated guide to reproducible data science: https://the-turing-way.netlify.com
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Some definitions

<table>
<thead>
<tr>
<th>Analysis</th>
<th>Data</th>
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<tbody>
<tr>
<td>Same</td>
<td>Same</td>
<td>Reproducible</td>
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<td>Different</td>
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<td></td>
<td>Different</td>
<td>Generalisable</td>
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The Turing Way, Chapter 2: Reproducibility [https://the-turing-way.netlify.com/reproducibility/03/definitions.html](https://the-turing-way.netlify.com/reproducibility/03/definitions.html) @eLifeInnovation #OAI11 #TheTuringWay
Reproducing results from a paper is difficult

Hyperparameters Revelio!
Stochastic Gradient Descendo!

What are you doing? I'm trying to reproduce the results from the latest DeepMind paper.

So far none of my spells seem to be working. I think I may need to invoke some even more powerful incantations.

Or, y'know, maybe just follow their description in the paper.

I'm in no mood for your jokes.

Silencio!

Image from Abstruse Goose: https://abstrusegoose.com/588
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It is a communication problem

Methods in 1979

Animals. This report is based on observations made on sixty-five Sprague-Dawley albino female rats. All animals were purchased from Hormone Assay Laboratories, Chicago, Illinois, and were ovariohysterectomized at least 2 weeks before the beginning of experimentation. During the course of behavioural observation, they were housed singly in a controlled environment at 24 °C with a reversed 12 hr light-dark cycle (lights off at 9 a.m.). Free access to laboratory chow and water was allowed at all times.

Preparation. The animals weighed between 260 and 320 g at the time of surgery. They were anesthetized with intraperitoneal Nembutal (35 mg/kg body wt.), and their heads were secured in a Kopf stereotaxic frame such that the skull was between the bregma and lambda. Cranietomy was made in the parietal area, and the dura was incised while preserving the sagittal sinus.

Monopolar electrodes were constructed from 10% iridium-platinum wire 175 μm thick, coated with Teflon except for the cut tip. Impedance of each electrode was 25-27 kΩ at 1 kHz. In forty-eight among sixty-five animals, implantation of the electrodes was made bilaterally, aiming for the rostral part of the v.m.n. with the stereotactic coordinates: 2-6 mm posterior (P) to the bregma, 0-6 mm lateral (L) to the mid line and ±5 mm deep (D) from the surface of the dura. In the remaining seventeen animals, electrodes were implanted bilaterally in either the medial preoptic area (nine rats), medial thalamic nuclei (four rats), or the cerebellar cortex. Stereotaxic co-ordinates for these sites were: (1) medial preoptic area: P 0-6, L 0-6, D 7-8; (2) medial thalamic nuclei: P 4-0, L 0-5, D 7-5; (3) cerebellar cortex: P 9-0, L 1-0, D 2-5. Indifferent electrodes were made from strands of uninsulated stainless steel wire wrapped around jeweller’s screws placed in the frontal bone. Electrodes were soldered to Amphenol pins, and fixed to the skull with dental cement.

Stimulation and testing procedure. Each animal received a subcutaneous injection of either 5 or 10 μg caerulein benzene in sesame oil on the day of the operation. Screening tests with bilateral stimulation of v.m.n. were made on day 4 (day of injection = day 0), on which the animals were recovered from the operation and displayed weak lordosis in response to manual cutaneous stimulation of the flanks followed by the ramp-tail base-perineum region (Pfaff, Montgomery & Lewis, 1977). The varying dosage of caerulein of 5 or 10 μg was found not to result in a significant difference either in the lordosis score or quotient, so the data are combined in appropriate categories of pre- and post-stimulation.

In the animals in which facilitation of lordosis was obtained in the screening, electrical stimulation was repeated under a variety of experimental conditions. Systematic analyses were

Methods in 2019

Materials and methods

Animals

In total, 89 male and female Long-Evans Tyrosine hydroxylase (Th)-Cre- rats (hemi-zygous Cre-) (Witten et al., 2011; Mahler et al., 2019) and wildtype (WT) littermates were used for this study. Subjects were at least 3 months of age at the start of the experiment and were single- or paired-housed in standard Plexiglas cages on a 12 hr/12 hr light/dark cycle. Animals were maintained at ~85% of their free-feeding weight during behavioral procedures. All experimental procedures that involved rats were approved by the UC Irvine Institutional Animal Care and Use Committee and were in accordance with the National Research Council Guide for the Care and Use of Laboratory Animals.

Apparatus

Behavioral procedures took place in sound- and light-attenuated Med Associates chambers (St Albans, VT, USA; ENV-007). Individual chambers were equipped with two retractable levers (Med Associates; ENV-112CM) positioned to the left and right of recessed food cup. Grain-based dustless precision pellets (45 mg, BioServ, Frenchtown, NJ, USA) were delivered into the cup using a pellet dispenser (Med Associates; ENV-203M-4D). Sucrose solution (20% wt/vol) was delivered into the cup with a syringe pump (Med Associates; PHM-100). A photobeam detector (Med Associates; ENV-254-CB) positioned across the magazine entrance was used to record food-cup approaches. Chambers were illuminated by a houselight during all sessions.
Containers: reproducible computing environments

A. CURRENT SYSTEM

Author’s Local Machine

Mac OS 10.10.5
R 3.1.3
Hgu133plus2 v18
HeLa dataset
Source Code

223 Significant Genes

Reader A

Ubuntu 14.04
R 3.2.4
Hgu133plus2 v19
HeLa dataset
Source Code

228 Significant Genes

Reader B

Mac OS 10.10.4
R 3.3.0
Hgu133plus2 v20
HeLa dataset
Source Code

227 Significant Genes

B. CONTAINER-BASED APPROACH

Authors build Docker Image

Mac OS 10.10.5

Docker

R 3.2.4
Hgu133plus2 v18
HeLa dataset
Source Code

Release Docker Image

Readers

Ubuntu 14.04

Docker

R 3.2.4
Hgu133plus2 v18
HeLa dataset
Source Code

223 Significant Genes

Beaulieu-Jones & Greene, 2016: https://doi.org/10.1101/056473
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Binder: Github repo → Docker image

Turn a Git repo into a collection of interactive notebooks

Have a repository full of Jupyter notebooks? With Binder, open those notebooks in an executable environment, making your code immediately reproducible by anyone, anywhere.
Do we want to reproduce experiments?

- Irreproducible = not true?
- Re-execution can be expensive and environmentally unfriendly
- Is anything beyond computational reproducibility achievable?

We want experiments to be reproducible, we may not want to reproduce them.
The humanities pursue meaning beyond truth. Confirming that Van Gogh painted Sunset at Montmajour (truth) is only the beginning. Unearthing the cultural meaning of the work requires historical context and theorizing on its message, style, aesthetics — and what the work can tell us about the artist and his world (view). The coexistence of multiple valid answers and the value of their interaction disqualify replication as a viable quality criterion.

Resist calls for replicability in the humanities. Sarah de Rijcke & Bart Penders. doi: 10.1038/d41586-018-05845-z
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The sciences pursue meaning beyond truth. Confirming that the rat moved into a certain position (truth) is only the beginning. Unearthing the meaning of the behaviour requires experimental context and hypothesising on its motives, internal state and sensory experience—and what the data can tell us about rats’ emotions and behaviour (view). The coexistence of multiple valid answers and the value of their interaction disqualify replication as a viable quality criterion should encourage interrogation, reuse and incorporation.

Resist calls for replicability in the humanities. Sarah de Rijcke & Bart Penders. doi: 10.1038/d41586-018-05845-z
@eLifeInnovation #OAI11
Moving from reproduction to reuse and collaboration

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Reproducible document Stack (RDS): putting code and data back into scientific narration

elifesci.org/reproducible-example
Progressive enhancement: read, interrogate and reuse

The possibility of change of confidence introduces an apparent dissociation between accuracy and

https://www.elifesci.org/reprodoc
@eLifeInnovation OAI11
Progressive enhancement: read, interrogate and reuse

Figure 7

Many features are conserved between the mammalian nephron and planarian prostonephridia.

(A) Image of a young adult C. elegans and schematic depicting the twelve pairs of sensory neurons in the anterior amphid ganglia whose dendrites project to the nose of the animal where they detect sensory stimuli.

(B) Average GCaMP fluorescence change in young adult (day 1), wild-type sensory neurons in response to medium concentration (0.005% vol/vol) BZ stimulation. Shaded box indicates two minute BZ odor stimulation beginning at t = 10 s. The light color shading around curves indicates s.e.m. and numbers in parentheses indicate number of neurons imaged.

(C) Summary chart of the calcium responses of all amphid sensory neurons to low (0.0001% vol/vol), medium (0.005% vol/vol) and high (0.1% vol/vol) concentrations of BZ odor. This chart shows the composition of the C. elegans olfactory neural circuit and depicts a combinatorial

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Progressive enhancement: read, interrogate and reuse

Figure 7

observed that the response amplitude to the non-rewarded, trained stimulus was

Plot type

Scatter

X axis

Temp

Y axis

Sales

Ice Cream Sales

15
20
25

Temperature

100
200
300

250

126

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You can help

- Share your use case
- Provide feedback
- Learn about progress and opportunities to help

Sign up: [elifesci.org/RDSupdates](elifesci.org/RDSupdates)

This will take you to a form asking for your consent to be added to a mailing list for bi-monthly emails with updates about this project, including calls for contributions and feedback.

Open-source community call, June 24, 4pm BST: [elifesci.org/os-community](elifesci.org/os-community)
Questions?

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Twitter: @eLifeInnovation / @emmy_ft
Labs:elifesci.org/labs